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Optimal Scaling of the Inverse Fraunhofer Diffraction Particle Sizing Problem: Analytic Eigenfunction Expansions

Abstract

There are many possible strategies for sampling the near-forward scattering pattern produced by a field of large particles and for subsequently solving the inverse problem in order to obtain an estimate of the particle size distribution. In a previous paper (*Part. Char.* Vol. 5, pp. 128-133, 1988) an optimally scaled formulation of the problem was derived based on consideration of condition numbers of the linear system obtained through numerical quadrature of the governing Fredholm integral equation. Here we consider "scaling" of the problem to involve selection of the parameters under control of the instrument designer (e.g. the number, angular positions, and aperture geometries of the detectors and the number, positions, and widths or weighting functions of the discrete size classes). Since the many numerical/analytical schemes for solving for the size distribution given a finite number of scattering measurements are fundamentally very similar, optimal scaling of the problem will improve the performance of the instrument regardless of the selected computational inversion algorithm.

In this paper we consider the analytic eigenfunction expansion method of solving the inverse Fraunhofer diffraction problem, and in particular how the scaling strategy affects the inversions. The eigenfunctions and associated eigenvalues for the diffraction problem (assuming infinite support) are derived in terms of two (variable) scaling parameters which describe the detector geometry and the size class configurations. It is shown that the rate of decrease of the eigenvalue spectrum with generalized frequency is minimized for the same scaling parameters ($a=2$, $b=2$) which optimized the condition numbers of the linear system. (A slower decrease in the eigenvalue spectrum indicates that the inversions will be less susceptible to corruption by noise, i.e. more stable). This optimal scaling study indicates, as was the case for the condition number analysis of the discrete linear system, that the particle size distribution solution should be on an area basis as $n(D)D^2$ and the scattering measurements should provide $i(\theta)\theta^2$.

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Optimal Scaling of the Inverse Fraunhofer Diffraction Particle Sizing Problem: Analytic Eigenfunction Expansions

In a previous paper Hirleman [1] formulated the integral equation governing the inverse Fraunhofer diffraction particle sizing problem as follows:

$$i_a(\theta) = \int_0^\infty [\, I_{inc}\lambda^2 / 4\pi^2 \,] \, [\, J_1^2(\alpha\theta) / (\alpha^{b-2}\theta^{2-a}) \,] \, n_b(\alpha) \, d\alpha \qquad (1)$$

where: $i(\theta)$ is the scattering intensity (W/sr) at a small forward angle θ; I_{inc} is the irradiance (W/m^2) of the incident beam (assumed uniform); α is the nondimensional particle size parameter equal to the particle circumference divided by the wavelength λ of the incident radiation ($\pi D/\lambda$); D is the particle diameter; $n(\alpha)$ is an unnormalized particle frequency distribution such that $n(\alpha)d\alpha$ is the number of optically-sampled particles in the optical beam with sizes between α and $\alpha + d\alpha$; J_1 is a Bessel function of first kind and first order; and a and b are constants where:

$$i_a(\theta) = i(\theta)\theta^a \qquad (2)$$

$$n_b(\alpha) = n(\alpha)\alpha^b \qquad (3)$$

Equation (1) assumes that Fraunhofer diffraction theory adequately describes the scattered light signature for the angles θ of interest and that multiple scattering is negligible. The diffraction assumption is satisfied generally when the angles θ are small, the particles are large compared to the wavelength, and the refractive index of the particles relative to the surroundings is not very close to unity. Finally, Eq. (1) neglects coherent scattering effects, i.e., assumes a very large number of randomly positioned particles are optically sampled. Now the scaling of the problem, which is the under auspices of the instrument designer, involves selection of parameters a and b and the number and orientations of detectors where measurements of $i_a(\theta)$ will be obtained. The measurements are used in the inverse problem, i.e. solving for $n_b(\alpha)$ in Eq. (1) using measured $i_a(\theta)$. Writing Eq. (1) in a more general integral equation form:

$$i_a(\theta) = I_{inc}\lambda^2 / 4\pi^2 \int_0^\infty k(\alpha,\theta) \, n_b(\alpha) \, d\alpha \qquad (4)$$

where $k(\alpha,\theta)$ is the kernel of the integral equation and by inspection of Eq. (1):

$$k(\alpha,\theta) = J_1^2(\alpha\theta) / (\alpha^{b-2}\theta^{2-a}) \tag{5}$$

Now McWhirter and Pike [2] formulated a solution scheme to Fredholm integral equations such as Eqs. (1) and (4) which applies for cases where the kernel function $k(\alpha,\theta)$ is a function of only the product of the two variables, i.e. $k = k(\alpha\theta)$. With this requirement we see from Eq. (5) that:

$$2 - a = b - 2 \tag{6}$$

or:

$$a + b = 4 \tag{7}$$

and we have lost one degree of freedom in scaling the problem as a and b are no longer independent. Equation (7) is the same condition for which the linear system produced by numerical quadrature of Eq. (1) takes the Toeplitz form as discussed by Hirleman [1]. If we define a new independent scaling parameter δ as:

$$\delta \equiv 2 - a = b - 2 \tag{8}$$

Then Eq. (1) becomes:

$$i_{2-\delta}(\theta) = I_{inc}\lambda^2 / 4\pi^2 \int_0^\infty k_\delta(\alpha\theta)\, n_{\delta+2}(\alpha)\, d\alpha \tag{9}$$

where:

$$k_\delta(\alpha\theta) = J_1^2(\alpha\theta) / (\alpha\theta)^\delta \tag{10}$$

The eigenfunctions ψ_ω and associated eigenvalues λ_ω of the kernel, if they exist, are defined by:

$$\lambda_\omega\, \psi_\omega(\theta) = \int_0^\infty k(\alpha\theta)\, \psi_\omega(\alpha)\, d\alpha \tag{11}$$

where ω is a continuous generalized frequency. Thus any components of the solution function $n_b(\alpha)$ which can be expressed in terms of the eigenfunctions ψ_ω of k will be passed through the integral operator intact but scaled by the associated eigenvalue λ_ω. In that case the inversion of the integral equation would be performed by expanding the measured scattering signature $i_{2-\delta}(\theta)$ in a series of the eigenfunctions. The eigenfunction components with significant amplitudes would then be used to synthesize the solution function after scaling by the appropriate eigenvalues. Now if the following integral of the kernel k is bounded:

$$\int_0^\infty |k(x)|\, x^{-1/2}\, dx < \infty \tag{12}$$

then a continuum of real eigenfunctions exist and have been found using Mellin transforms by McWhirter and Pike [2] as:

$$\psi_\omega^+(\theta) = \mathrm{Re}[\phi_\omega(\theta)] \tag{13}$$

$$\psi_\omega^-(\theta) = \mathrm{Im}[\phi_\omega(\theta)] \tag{14}$$

where the corresponding real eigenvalues are:

$$\lambda_\omega^\pm = \pm\, |\, K((1/2) + i\omega)\, | \tag{15}$$

and where the Mellin transform $K(s)$ of $k(x)$ is defined by:

$$K(s) \equiv \int_0^\infty x^{s-1}\, k(x)\, dx \tag{16}$$

and:

$$\phi_\omega(\theta) = \frac{\theta^{-(1/2)-i\omega}\ \sqrt{K((1/2) + i\omega)}}{\sqrt{(\pi\, |\, K((1/2) + i\omega)\, |)}} \tag{17}$$

It is also sufficient to consider only $\omega > 0$ as pointed out by McWhirter and Pike [2] and Viera and Box [3].

Now we will need to obtain the Mellin transform defined in Eq. (16) of the kernel family of Eq. (10) as:

$$K_\delta(s) = \int_0^\infty x^{s-1}\, J_1{}^2(x) / x^\delta$$

$$= \frac{(1/2)^{\delta-s}\,\Gamma(\delta+1-s)\,\Gamma(1-(\delta/2)+(s/2))}{2\,\Gamma^2(1+(\delta/2)-(s/2))\,\Gamma(2+(\delta/2)-(s/2))} \tag{18}$$

We can then calculate the eigenvalue spectrum from Eq. (17) which requires:

$$K_\delta((1/2)+i\omega) = \frac{(1/2)^{\delta-(1/2)-i\omega}\Gamma(\delta+(1/2)-i\omega)\,\Gamma((5/4)-(\delta/2)+(i\omega/2))}{\Gamma^2((3/4)+(\delta/2)-(i\omega/2))\,\Gamma((7/4)+(\delta/2)-(i\omega/2))} \tag{19}$$

which, for δ=2 simplifies to Eq. (3.3) of Bertero and Pike [4].

Before going further we must also consider the values of δ for which the kernel k_δ of Eq. (10) satisfies Eq. (12). Substituting k_δ for k in Eq. (12) results in the condition:

$$\int_0^\infty J_1{}^2(x)\, x^{-(1/2)-\delta}\, dx < \infty \qquad (20)$$

Convergence of this integral requires that $3 > (-1/2-\delta) > 0$ or:

$$2.5 > \delta > -0.5 \qquad (21)$$

For this paper we consider integer values for δ of 0, 1, and 2 which give physically meaningful properties to the functions $i_{2-\delta}$ and $n_{\delta+2}$ as shown in Table I.

Table I

δ	$i_{2-\delta}(\theta)$	Detector	$n_{\delta+2}(\alpha)$	Form of $n_{\delta+2}(\alpha)$
2	$i(\theta)$	Linear Array	$\alpha^4 n(\alpha)$	
1	$i(\theta)\theta$	Constant Δr Rings	$\alpha^3 n(\alpha)$	Volume distribution
0	$i(\theta)\theta^2$	Log-scaled Rings	$\alpha^2 n(\alpha)$	Area distribution

Now an indication of the quality of the scaling of an inverse problem is the rate at which the eigenvalues roll off with increasing frequency ω. This is true because the solution to Eq. (9) based on eigenfunction expansions will be:

$$n_{\delta+2}(\alpha) = \int_0^\infty n_{\delta,\omega}{}^+\, \psi_\omega{}^+(\alpha)\, d\omega + \int_0^\infty n_{\delta,\omega}{}^-\, \psi_\omega{}^-(\alpha)\, d\omega \qquad (22)$$

where:

$$n_{\delta,\omega}{}^\pm = i_{\delta,\omega}{}^\pm / \lambda_\omega{}^\pm \qquad (23)$$

and:

$$i_{\delta,\omega}{}^\pm = \int_0^\infty i_{2-\delta}(\theta)\, \psi_\omega{}^\pm(\theta)\, d\theta \qquad (24)$$

It can be seen from Eq. (23) that as the eigenvalues $\lambda_\omega{}^\pm \to 0$, the $n_{\delta,\omega}{}^\pm$ and therefore the solution grows without bound. The illconditioned nature of the problem would then be manifested

as small perturbations in $i_{\delta,\omega}{}^{\pm}$, for example due to measurement errors in $i_{2-\delta}(\theta)$, would be magnified greatly at frequencies ω where the $\lambda_\omega{}^{\pm}$ are small. For that reason it is necessary to truncate the integrations in Eq. (22) at some finite value ω_{max} of the generalized frequency. In that case we approximate the solution as:

$$n_{\delta+2}(\alpha) \cong \int_0^{\omega_{max}} n_{\delta,\omega}{}^{+} \psi_\omega{}^{+}(\theta)\, d\omega + \int_0^{\omega_{max}} n_{\delta,\omega}{}^{-} \psi_\omega{}^{-}(\theta)\, d\omega \tag{25}$$

In that case, components of $n_{\delta+2}(\alpha)$ at frequencies above ω_{max} are inaccessible to the experiment.

Now there is a tradeoff between a desire to make ω_{max} as large as possible in order to minimize the truncation error in Eq. (25) but at the same time keep the solution stable by not including frequencies with small eigenvalues. For that reason the behavior of the eigenvalue spectrum, shown in Fig. 1, is very important. For the possible values $\delta = 0, 1, 2$ the optimal value is clearly $\delta = 0$ which gives the slowest rolloff of $\lambda_\omega{}^{\pm}$. The value $\delta = 0$ corresponds to $a = b = 2$, that is a solution on a particle area basis using log-scaled ring detectors. This result is identical to that obtained by Hirleman [1] using a condition number analysis on the linear system produced by numerical quadrature of Eq. (9).

The asymptotic behavior of the eigenvalue spectrum is interesting as well, and taking the limit of Eq. (19) as $\omega \rightarrow \infty$ and using Eq. (15) we obtain:

$$\lim_{\omega \to \infty} \lambda_\omega{}^{\pm} = \omega^{-\delta-1} \tag{26}$$

Again, the value of $\delta = 0$ is the best of the those considered, where in the limit of large ω the eigenvalues are proportional to ω^{-1}.

Some Comments on Instrument Design

It is clear from the previous analysis that the parameter δ, and in turn the instrument scaling parameters a and b, control the nature of the numerical inversion based on eigenfunction expansions. Thus the stability, the information content, and other measures of the performance of an inverse scattering solution based on analytic eigenfunctions is determined by the selection of parameters a and b. This has also shown to be the case for inversion of the linear system produced by numerical quadrature of Eq. (9), and it is expected to hold for a singular function expansion [3,5] as well. It is crucial, then, to understand constraints on the values of a and b which might be implemented in practice. Now an underlying assumption governing the validity of the condition number as a measure of inversion stability[1] and of the scheme proposed here for truncating the eigenfunction series approximation using a noise-based criterion is that of white noise. If, for example, the noise produced by a detector were constant per unit area of active detector surface, then the white noise assumption would only be true for $a = 0$ as pointed out by Bertero and Pike

[4,5]. This forces the instrument (for a product kernel or Toeplitz matrix form) to b = 4 and, in turn, $\delta = 2$. Clearly it would be better to have the freedom to select a detector geometry based on optimizing the expected numerical performance of the inverse problem and force the detector to conform rather than vice versa.

One possible approach is to use the optical system shown in Fig. 2 as developed by Hirleman and Dellenback [6], where the detector area (noise-producing) does not depend on the collection aperture for the discrete detection angles θ. The optical system of Fig. 2 uses a transmission-mode spatial light modulator to create programmable mosaic arrays (of arbitrary shape) of detector openings which pass selected portions of the scattering signature on through to the field lens and single detector. While the parallel, simultaneous detection capabilities are lost with a system as in Fig. 2, the potential for intelligent, programmable detector arrays overrides that disadvantage.

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Nomenclature

a	instrument scaling parameter (nondimensional) for particle size distribution function basis
b	instrument scaling parameter (nondimensional) for scattering intensity moment
D	particle diameter (m)
$i(\theta)$	scattering intensity (W/sr) at angle θ
I_{inc}	incident irradiance (W/m2)
J_1	Bessel function of first kind and first order
$k(\alpha,\theta)$	general kernel function for the integral equation
$k(\alpha\theta)$	product-form of the kernel k
K	Mellin transform of the kernel function k
α	particle size parameter, $\pi D/\lambda$
δ	instrument scaling parameter (nondimensional) which arises when k is a product kernel.
θ	scattering angle measured from the optical axis
λ_ω	eigenvalue corresponding to frequency ω
ψ_ω	eigenfunction for the kernel of the integral equation
ω	generalized frequency

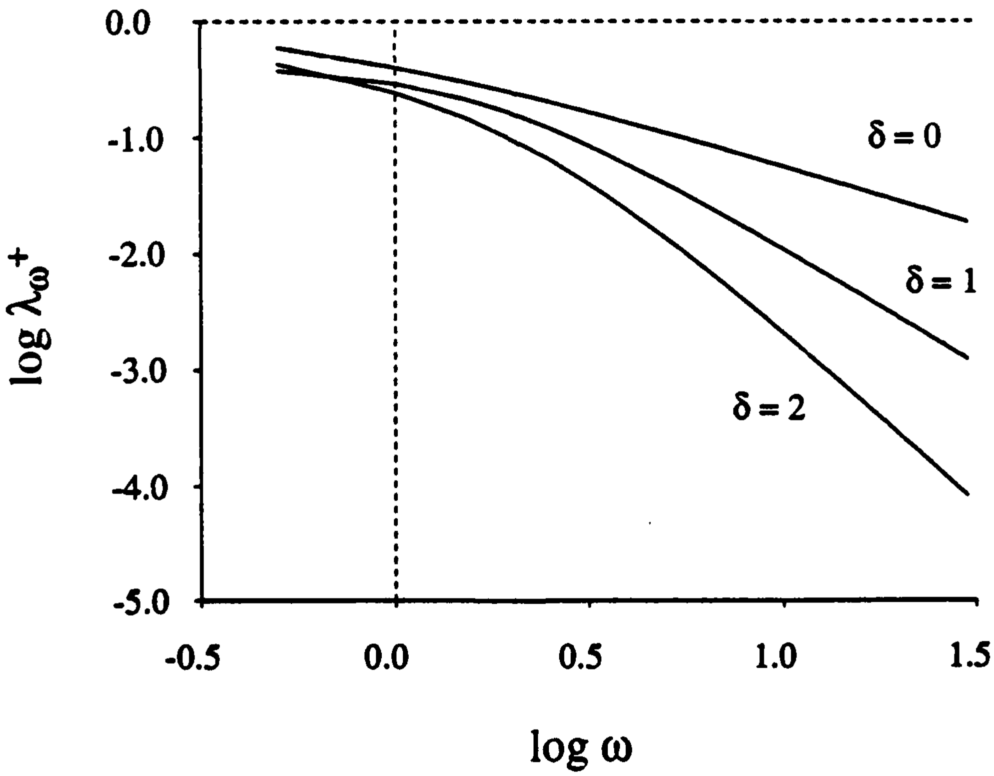

Figure 1. Plot of the eigenvalue spectrum λ_ω^+ of the Fraunhofer diffraction integral equation for the kernel described by Eq. (19). The spectra for three values of the scaling parameter δ are shown. The asymptotic behavior of the curves are described by Eq. (26).

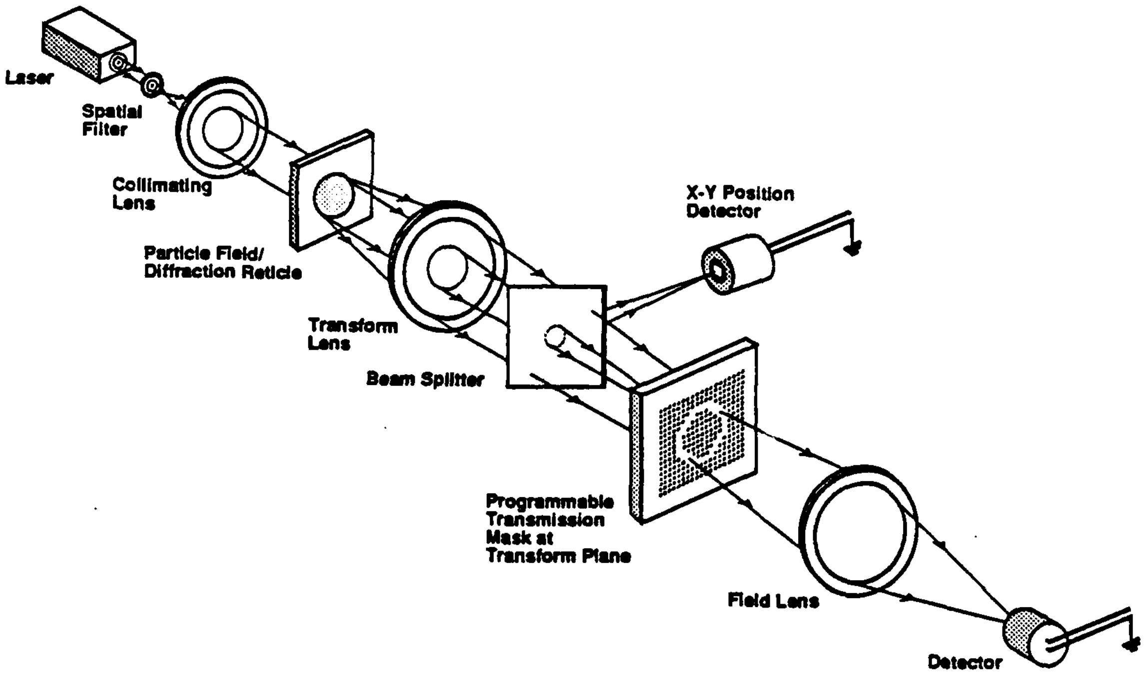

Figure 2. Schematic of a laser diffraction particle sizing instrument where a spatial light modulator operated as a programmable transmission mask has been included to provide for on-line, adaptive configuration of the detector collection apertures. Annular ring openings are created in the SLM at the transform plane by setting the pixels to transmit or block the incident polarized light. The rings are created concentric with the optical axis as measured in real-time by the x-y position detector shown. The field lens collects all light passing through the SLM and passes it the the detector, and the system is sequenced through a set of rings.